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Förster resonant energy transfer between CdSe nanocrystals: An empirical pseudopotential/transition density cube approach<sup>1</sup> JOSHUA SCHRIER, LIN-WANG WANG, Lawrence Berkeley National Laboratory — We study the energy transfer between semiconductor nanocrystal dots and rods of CdSe using a semiempirical pseudopotential method (SEPM) description of the electronic structure of the nanocrystals, followed by evaluation of the Coulombic contribution to the energy transfer evaluated using the transition density cube (TDC) method. Our results are compared to the dipole-dipole theory of Förster to characterize the effects of nanocrystal shape, distance, and orientation. In agreement with previous effective-mass and tight-binding studies, we find that the coupling between spherical nanocrystals is well described by the Förster model. In contrast, we find that rod-shaped nanocrystals display more complicated behavior, which may be relevant to exciton migration in all-inorganic nanorod-based photovoltaic devices.

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Joshua Schrier Lawrence Berkeley National Laboratory

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